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By

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Numerical Model of Dispersion of Atmosphere Pollution Within Urban Agglomeration (M. Uliasz)

Introduction. One of the most frequent of air pollutants emitted in urban environments is sulfur dioxide. Oxidation processes in the atmosphere are the cause of sulfur dioxide turning into sulfuric acid. As a result of chemical reactions with 1 mg of SO_2, 1.531 mg of H_2SO_4 occurs. The acceptable concentrations for safety zones are about 3 times stronger for sulfuric acid than for sulfur dioxide, or that same quantity of sulfur in the form of H_2SO_4 in free air is about a 4.5 times greater threat to the environment than in the form of sulfur dioxide.

The paper presents a numerical model of the dispersion and conversion of sulfur dioxide emitted from an urban area. Using a two-dimensional diffusion model makes it possible to find, besides the SO_2 decomposition concentration, the decomposition concentration of sulfuric acid also as one of the end products of the oxidation of sulfur dioxide.

Diffusion Model. The model considered in pollution dispersion is given by the equation

$$u \frac{\partial \vec{S}}{\partial x} = \frac{\partial}{\partial z} K \frac{\partial \vec{S}}{\partial z} + \vec{f} \qquad (1)$$

with boundary conditions

$$x = 0, \vec{S} = 0, \tag{2}$$

$$z = 0, K\frac{\partial \vec{S}}{\partial z} = \vec{v}\vec{S} - \vec{Q}, \tag{3}$$

$$z = H, \vec{S} = 0, \tag{4}$$

where $\vec{S} = \begin{pmatrix} S_1 \\ S_2 \end{pmatrix}, \vec{f} = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, \vec{v} = \begin{pmatrix} v_1 & 0 \\ 0 & v_2 \end{pmatrix}, \vec{Q} = \begin{pmatrix} Q_1 \\ 0 \end{pmatrix},$

$S_i = S_i(x, z)$ is the pollution concentration, f_i is the volumetric intensity of the pollution source, v_i is the pollution absorption rate by the GROUND, Q_1 is the pollution emission from a unit of surface, whereby when $i = 1$ the quantity reaches SO_2, and when $i = 2$ the quantity reaches H_2SO_4, $u = u(z)$ the velocity of air, $K = K(z)$ the vertical turbulence coefficient, H is the height of the mixing layer.

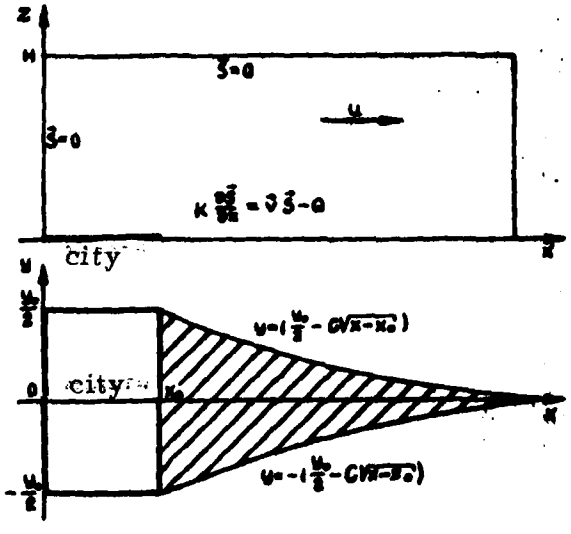

Fig. 1. Field and boundary conditions of the model.

The field of action of the model is presented in Figure 1, assuming that from the surface of the city sulfur dioxide is emitted and with that, it is assumed that pollution does not take place on the windward side of the source of emission.

Where $z=H$, a second variant of the boundary condition was tested also:

$$\frac{\partial \vec{S}}{\partial z} = 0 \qquad (9)$$

With the proposed height of the mixing layer $H=1,000$ m, the results from the model, with different boundary condition variants (4) and (5), were practically identical.

The model takes into consideration the pollution absorption by the ground. The absorption speed is understood as the relationship of the vertical turbulent pollution flow to its concentration at the surface of the ground. It is assumed that sulfuric acid is absorbed by the ground identically like sulfur dioxide, consequently $v_1=v_2$. In open space it is granted that the absorption rate is equal to 1 cm /s /3/, while for the city it is conventionally 3 times greater.

The two-dimensional diffusion model defines the decomposition of pollution concentration emitted by the surface source infinitely extending in the direction of the y axis. In the case of the town--a source having finite

measurements--the model describes the concentration only in the zone in which the concentrations are not dependent on the y_o dimension of the emission source (the area is marked off in Fig. 1). This zone is designated by the inequality

$$-(y_o/2 - C\sqrt{x - x_o}) \leq y \leq (y_o/2 - C\sqrt{x - x_o}) \qquad (6)$$

where $C = 3\sqrt{2K_y/u}$, K_y -- the turbulence coefficient in the direction of the y axis.

The length of the validity zone of the model in the direction of the wind is usually about 4 to 5 times greater than the width of the emission source of y_o. The model gives the highest values of pollution concentration from those that take place. Beyond the limits of the field defined by condition (6) the results of the model will be exaggerated.

In the model considered it is assumed that the only product of the sulfur dioxide oxidation is sulfuric acid. The SO_2 loss in equation (1) is shown by f_1, while the appearance of H_2SO_4 is taken care of by f_2, whereby we get: $f_2 = -1.531f_1$. Most often it is agreed that the loss of sulfur dioxide is proportional to its concentration, so called $f_1 = -kS_1$. In this case the time of half loss of pollution is $\tau_{1/2} = 1n2/k$. In the above supposition the calculations for small wind velocities give relatively high values of H_2SO_4 concentrations at great distances from the source of emission, even higher than

from SO_2 concentrations [1]. Under actual conditions such situations are not observed. In accepting the hypothesis that the conversion rate of SO_2 into H_2SO_4 depends on the sulfur dioxide concentration, the model uses the following form of conversion function [1]:

$$f_1 = -(k_1 S_1 + k_2 S_1^2 + k_3 S_1^3) \qquad (7)$$

In this supposition the time of half loss of SO_2 is a function of its concentration:

$$\tau_{1/2} = \frac{\ln 2}{k_1 + k_2 S_1 + k_3 S_1^2} \qquad (8)$$

The conversion factors k_1, k_2, k_3 were selected in order to retain proportions between the concentration of H_2SO_4 and SO_2, occurring in actuality.

In accepting that $k_1 = 4 \cdot 10^6\ s^{-1}$, $k_2 = 2 \cdot 10^{-4}\ s^{-1}\ m^3\ mg^{-1}$ i $k_3 = 0{,}1\ s^{-1}\ m^6\ mg^{-2}$, for the concentration $SO_2 S_1 = 0.04$ mg $/m^3$, $\tau_{1/2} = 1$hr , and for the concentration $S_1 = 0.004$ mg $/m^3$ $\tau_{1/2} = 30$ hrs.

The numerical solutions of the diffusion equation make it possible to take into consideration arbitrary distributions of meteorological parameters. The wind velocity and turbulence factor are accepted in the model as functions of height over the surface of the earth z_1, coarseness of the base z_o and geostrophic wind velocity G:

$$u(z) = \frac{u_*}{\kappa} \ln \frac{z + z_0}{z_0} \qquad (9)$$

$$K(z) = \begin{cases} \kappa u_* (z + z_0) & \text{for } z \leqslant -200 \text{ m} \\ \kappa u_* (200 + z_0) \exp(-1{,}3\, z) & \text{for } z > 200 \text{ m} \end{cases}$$

The dynamic velocity u_* can be expressed by the Lettau formula [4]:

$$u_* = G \frac{0{,}16}{\lg Ro - 1{,}8}$$

where $Ro = G/(z_0 l)$ is Rossby's number, l is the Coriolis parameter, u is the Karman constant.

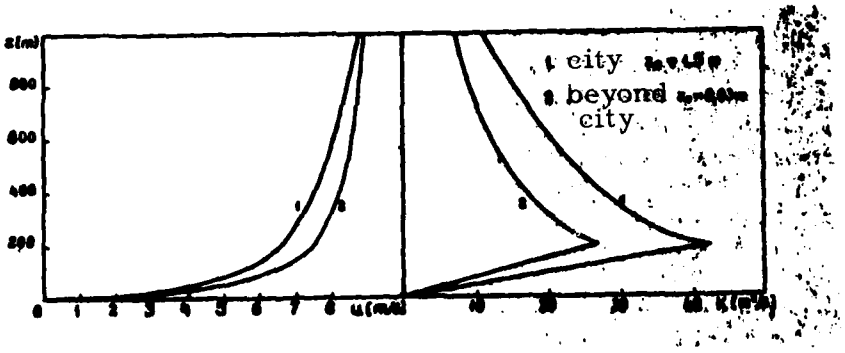

Fig. 2. Distribution of wind velocity and turbulence coefficient in the city and beyond the city for G=6 m/s.

For the urban area the parameter of courseness is $z_0 = 1.5$ m , and for the non-urban area $z = 0.03$ m. A fall in wind velocity and an increase in turbulence factor is attendant to an increase in the coarseness of the ground z_0 (Fig. 2.).

From the equation for continuity for the air

$$\frac{\partial w}{\partial z} + \frac{\partial u}{\partial x} = 0 \qquad (12)$$

we conclude that at the city limits, with a change in profile of wind velocity u, vertical movements appear which surround the air with the velocity w. In the model these movements were omitted since the value of the vertical air velocity w does not exceed 1% of the wind velocity u.

Equation (1) is solved numerically by a network method using the following differential scheme [6]:

$$u_k \frac{S_{j+1,k} - S_{jk}}{\Delta x} = \frac{K_{k+1/2}(S_{j+1,k+1} - S_{j+1,k}) - K_{k-1/2}(S_{j+1,k} - S_{j+1,k-1})}{\Delta z^2} + f$$

when k=2, ..., n-1, j=1, ..., m - 1.

Boundary conditions (2), (3), and (4) are approximated by the following differential equations:

$$\left.\begin{aligned} S_{1,j} &= 0 && k = 1, \ldots, n \\ S_{1,j} &= P_{1,j} S_{2,j} + R_{1,j} \\ S_{n,j} &= P_{2,j} S_{n-1,j} + R_{2,j} && j = 2, \ldots, m \end{aligned}\right\} \qquad (13)$$

To solve the differential scheme (12) with boundary conditions (13) the "progonki" method [5] is used which permits passing from quadratic equations (14) to a linear equation system (15).

$$A_{k,j+1} S_{k-1,j+1} - C_{k,j+1} S_{k,j+1} + B_{k,j+1} S_{k+1,j+1} = -F_{kj} \qquad (14)$$

$k = 2, \ldots, n-1; \quad j = 1, \ldots, m-1$

For the given j the solution sought is in the form

$$S_k = X_{k+1} S_{k+1} + Y_{k+1} \qquad k = n-1, \ldots, 1 \qquad (15)$$

where $X_2 = P_1, \quad Y_2 = R_1$

$$X_{k+1} = \frac{B_k}{C_k - X_k A_k}, \; Y_{k+1} = \frac{A_k Y_k + F_k}{C_k - X_k A_k} \quad k = 2, \ldots, n-1 \qquad (16)$$

and $$S_n = (R_2 + P_2 Y_n)/(1 - P_2 X_n) \qquad (17)$$

The "progonki" method is stabile if

$$A_k > 0, \; B_k > 0 \text{ i } A_k + B_k < C_k \qquad (18)$$

Analysis of Results. The model was tested for 3 variants of geostrophic wind velocity 3.6 and 10 m/s. Uniform emission of sulfur dioxide from the urban area was assumed, equal to 100 t/km^2/per yr.

Distributions of sulfur dioxide concentrations for different variants of geostrophic wind velocity are presented in Fig. 3a, b, c. An increase in wind velocity causes a definite fall in the concentration of pollution. With an increase in wind velocity individual isolines of concentration enclose smaller and smaller areas. Maximum concentrations of sulfur dioxide occur at the earth's surface at the leeward outskirts of the city (z=0, x=10 km.).

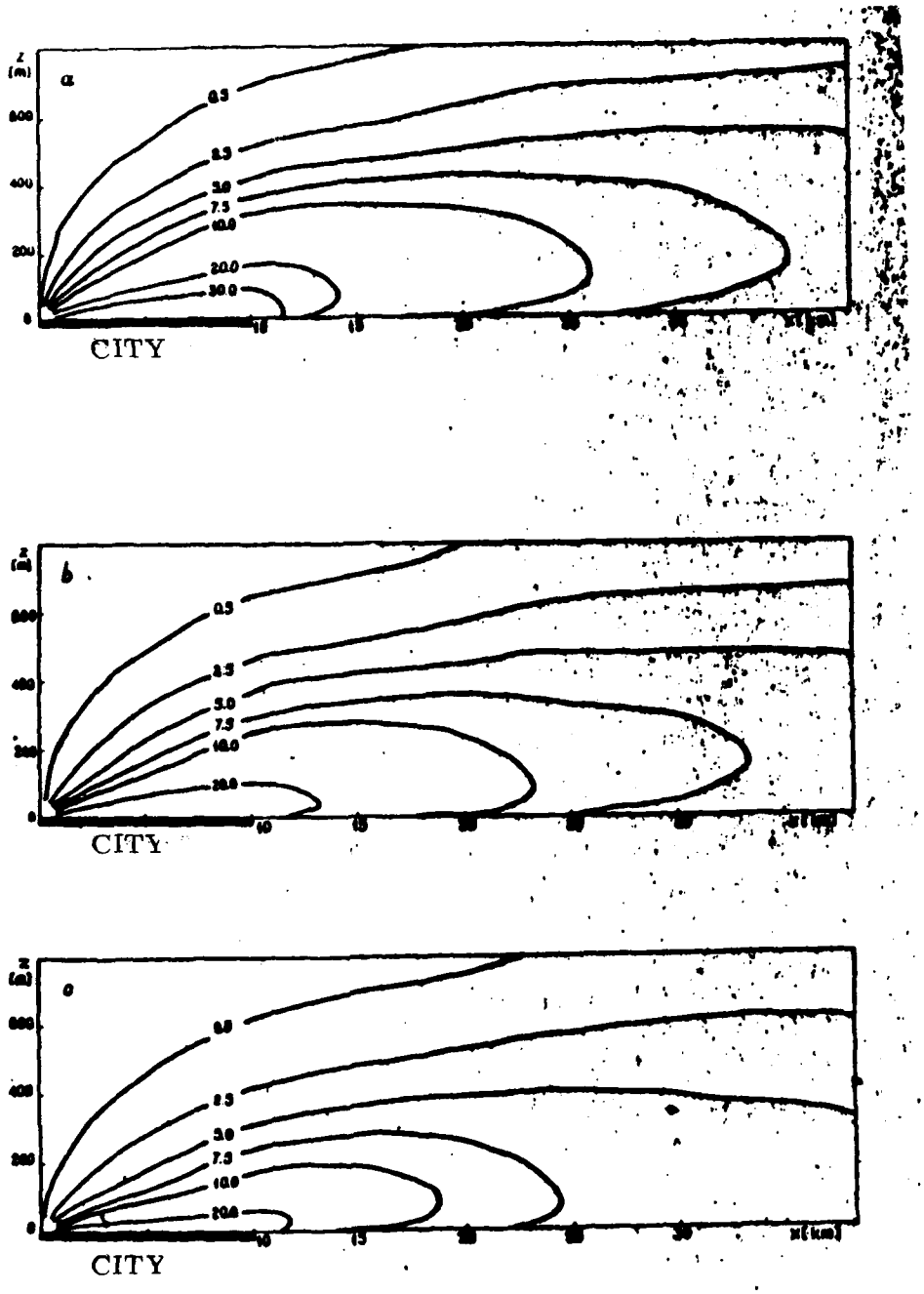

Fig. 3. Isolines of SO_2 concentration [$\mu g/m^3$]
a - $G = 3$ m/s; b - $G = 6$ m/s; c - $G = 10$ m/s

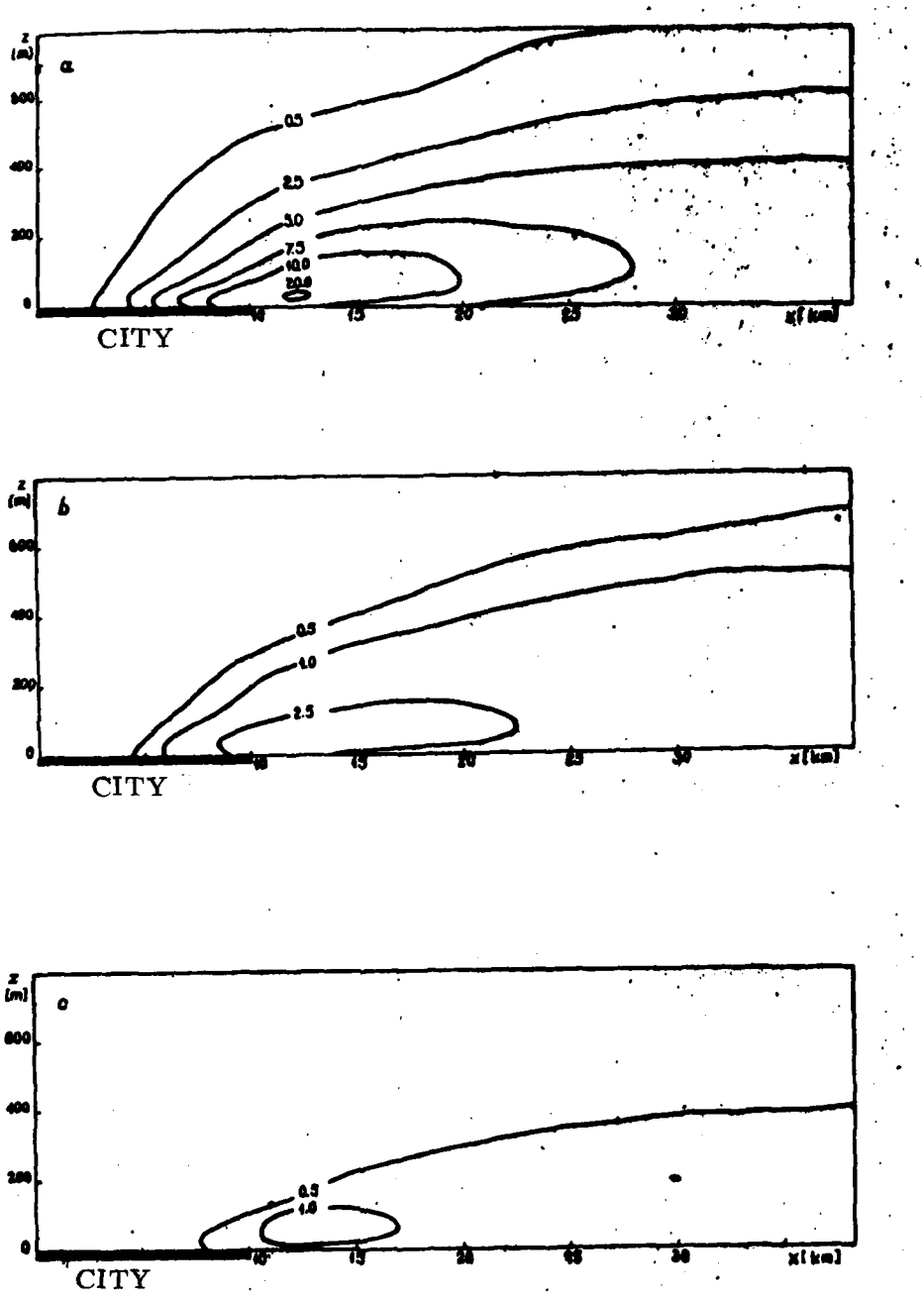

Fig. 4 Isolines of H_2SO_4 concentrations [$\mu g/m^3$]
a – $G = 3$ m/s; b – $G = 6$ m/s; c – $G = 10$ m/s

x [km] \ v [m/s]	3	6	10
2	0,0	0,2	0,0
4	0,6	0,2	0,1
6	2,0	0,6	0,4
8	3,9	1,2	0,8
10	5,8	1,9	1,1
12	28,4	8,9	4,7
14	30,9	10,6	5,4
16	31,8	11,4	5,7
18	32,4	11,9	5,9
20	32,5	12,2	6,0
22	32,7	12,6	6,2
24	33,0	12,9	6,4
26	33,6	13,3	6,6
28	34,1	13,7	6,8
30	34,7	14,1	7,0
35	35,8	14,9	7,4
40	36,7	15,6	7,9

Relationship of quantity of sulfur in the form of H_2SO_4 to summary quantity of sulfur when z = 0 m.

The effect of the increase in wind velocity on the fall of sulfuric acid concentration is even stronger than in the case of SO_2 (Fig. 4a, b, c).

The greatest H_2SO_4 concentrations occur at a certain height over the earth and are clearly displaced in the direction of the wind, in relation to the greatest concentrations of sulfur dioxide. An evident fall in the concentrations of both pollutants at the earth's surface (beyond the emission area in the case of SO_2) is connected with the absorption of the pollutants by the ground.

The ratio of the quantity of sulfur in the form os H_2SO_4 to the summary quantity of sulfur when z=0 retains, beyond the outskirts of the city, values approximately constant for the given wind velocity (Table). Benarie, Nonat, et al. [1] show that the values of this relationship are weakly dependent on the distance from the emission source and fluctuate from 5 to 23%. According to tests made by Hryniewicz [2] for Warsaw, the percent of sulfur in a sulfur aerosol, calculated in relation to the summary quantity of sulfur in gas and aerosol, amounts to 7 to 32% depending on the season of the year. The results of the model presented in the paper are, consequently, concurrent with the experimental data.

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